Manual for WAND² Event Filter and Sequential Fit

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I) Event Filtering:

WAND² is recording data in event mode. This means each neutron gets its individual timestamp.

In this section, we explain how to filter the data for neutrons with a certain timestamp (or any recorded parameter; for instance, temperature).

1) Go to File on the left upper corner and hit "Open Script" or Ctrl+O.

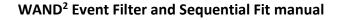
File	View	Interfaces	Help						
Ope	n Script			Ctrl+O	-				
Open Project									
Save	Script	Ctrl+S							
Save Script as									
Ope	n Recen	tly Closed S	cripts		•				
Gene	erate Re	covery Scrip	t						

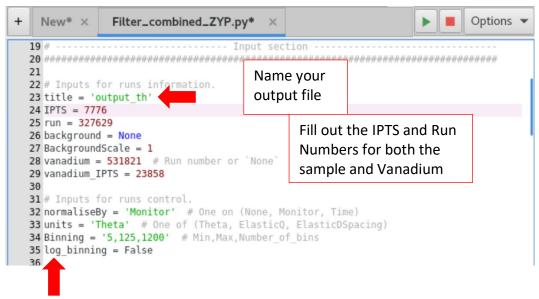
Follow the path data→HFIR→HB2C→shared→WANDscripts and locate

"Filter_combined_ZYP.py".

4	Q - 24-10-10-10-10	data	HFIR	HB2C	shared	WANDscripts	
	8						
wan	a2_sca_reauction.py					4.4 KB	тя нер
🛑 New	v						20 Feb
write	er.py					2.5 kB	7 Mar
write	er2.py					2.5 kB	7 Mar
📄 Old							9 Mar
work	karound_nuclear.py					1.1 kB	12 Apr
save	e_multiple_powder.py					1.1 kB	19 Apr
SCD	_MDE_Vana.py					1.4 kB	29 Apr
📁 scd							24 May
📄 Filte	r_combined_ZYP.py					6.9 kB	25 May
							2 Jun

 After the script has been loaded, go to the first paragraph of the script and fill out all the information: name of the output workspace, IPTS and Run Numbers for both your data and Vanadium (background), NormaliseBy, Units, Binning, and Sample Log that will be used to filter.





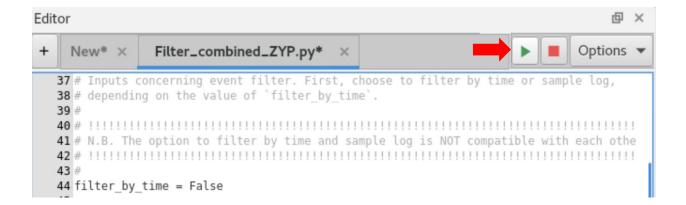
In the second paragraph, modify "normaliseBy", "units", and "Binning" if needed.

3) You can filter by time by typing "**True**" **OR** you can filter by Sample Log (only one option can be picked at once).

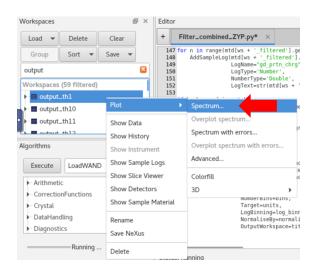
```
37 # Inputs concerning event filter. First, choose to filter by time or sample log,
38 # depending on the value of `filter by time`.
39 #
41 # N.B. The option to filter by time and sample log is NOT compatible with each othe
43 #
                                       Change "False" to "True"
44 filter by time = False
45
                                       to filter by time and modify
46 # Inputs concerning event filter by time.
                                       the next paragraph as
47 if filter by time:
                                       necessary.
     start_time = '0'
48
     stop_time = '100'
49
50
   time_interval = '10'
51
     unit of time = 'Seconds'
52
     time tolerance = 0
53
54 # Inputs concerning event filter by sample log.
55 LogName = 'HB2C:SE:SampleTemp'
                                          If using Sample Log, go to
56 LogValueInterval = 25
                                          "Show Sample Logs" and
57 MinimumLogValue = None
58 MaximumLogValue = None
                                          choose the Sample Log. To
59 log val tolerance = LogValueInterval / 2.0
                                          find the Sample Log, use
60 log change direction = 'Both'
                                          LoadWAND to upload the
61
                                          data, then right click on the
                                          workspace created and
                                          select "Show Sample Logs".
```

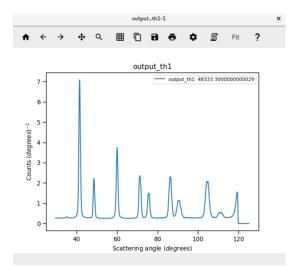
If filtering by Sample Log is chosen, it is not recommended to have more than 20 intervals for a reasonable time of processing (e. i. if the temperature runs from 100K to 600K, the maximum value for the interval would be 25K).

4) When finished, hit Run.

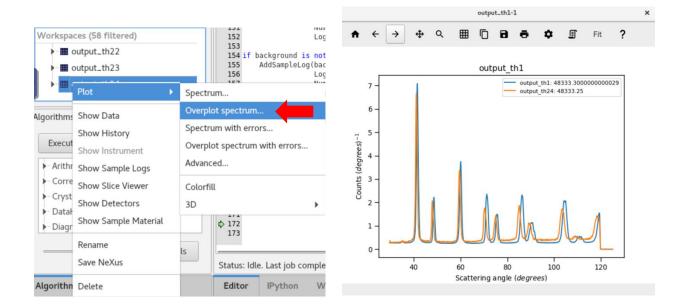


5) Once the script has finished running, the new output workspace (the one that was created in the previous step – default name is "output_th") can be accessed in the "Workspace" window. Right clicking on the first file to plot individually. You can also select to plot spectrum with error depending on your goal.

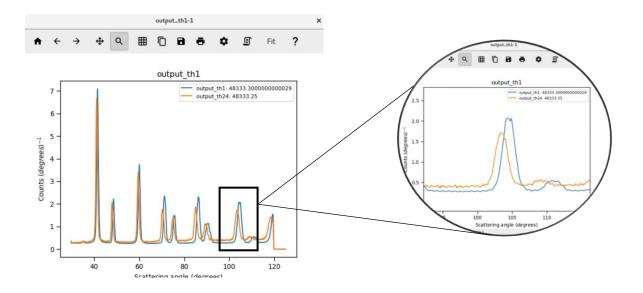




6) Right click on another file and select "Overplot spectrum".

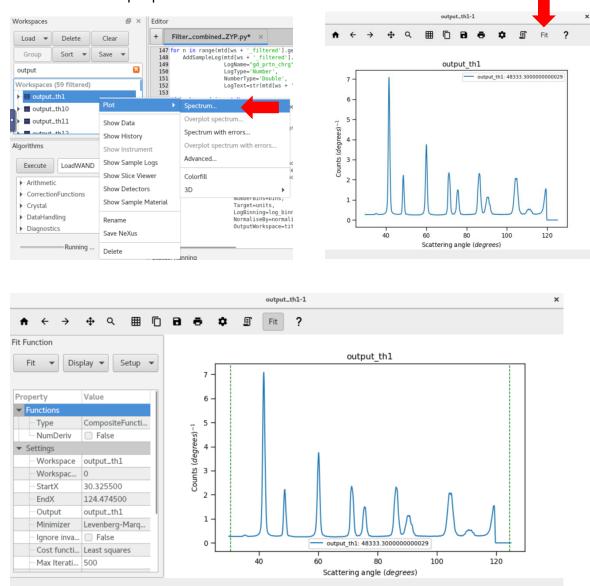


Click on the zoom to view an individual peak shift.



II) Fitting the peaks.

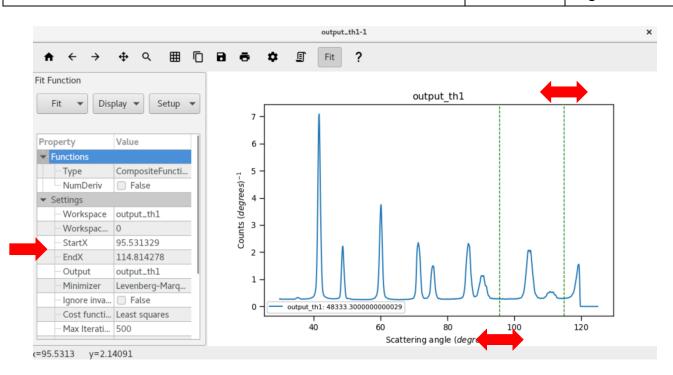
1) In this section, we will explain how to extract parameters from multiple data sets from event filtering. In order to fit the peaks, plot the folder ("**Spectrum**" or "**Spectrum with error**") and click on "**Fit**" on top a plot.



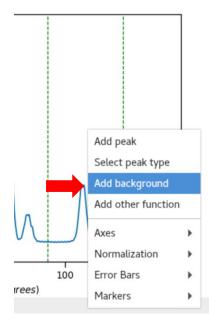
2) Move the green lines or enter the interval for fitting manually.

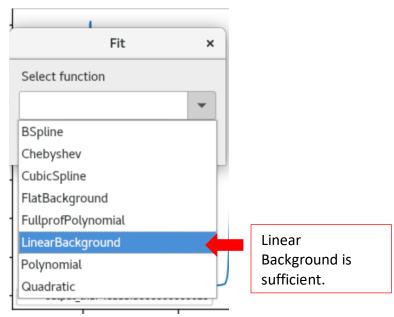




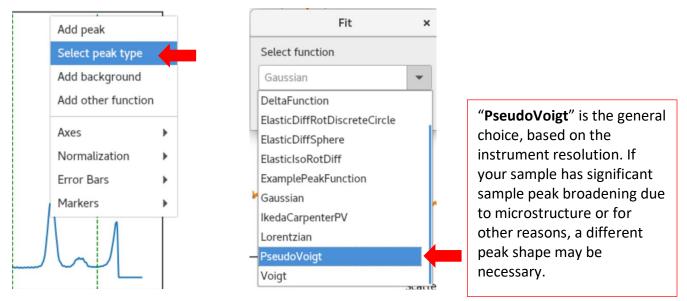


3) Right click on the peak to "Add background".

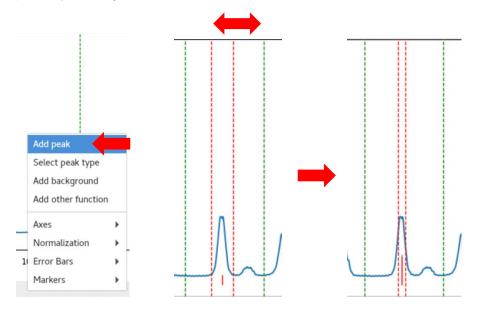




4) Right click on the peak to "Select peak type".

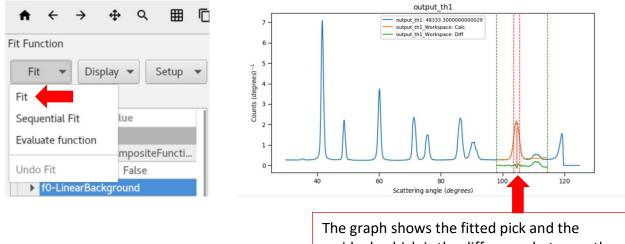


5) Right click and select "**Add peak**", click on the peak to fit and adjust the red lines to fit the peak by moving them.



- 6) There are two ways to fit the peak: you can either fit it individually or use sequential fit.
 - a. To fit, click on "Fit" and then select "Fit".





The graph shows the fitted pick and the residual, which is the difference between the fitted peak and the data.

b. For sequential fitting to fit multiple patterns sequentially using the same dialogue:

	1. 7 (10)	SequentialFit ×								
It is necessary modify the Log Value depending on the Sample Log		f0.A0 SourceName ainst log Output (Pass work		• to function	ve Type		•	-	Type" spaces should not be modified because they are used to create an output plot,
that was used on for data collection and in		kspace/File ut_th1	Period	Spectrum -1	WS Index 0	Range		Add workspaces	s	which is currently not implemented.
the script.	Period	1	- +	Spectrum	0	- +	• Sequen	Delete		
	?						F	it Cancel		

i. After that, click on "Fit" and then on "Sequential Fit".

ii. Click on "Add Workspaces".

				Mantid - Select workspace	×
	Sequentia	alFit	×		
arameter	f0.A0 👻	Curve Type Line	•	HB2C_327633_monitors	
og Value	SourceName			output_th1	
	gainst log 📃 Pass workspace index to funct				
Input	Output 🔲 Output Composite Members	Convolve Members		output_th10	
W	orkspace/File Period Spectrum WS I	ndex Range	Add workspaces	output_th11	
1 out	out_th1 -1 0		Add files	output_th12	
			Delete	output_th13	1
				output_th14	
Period	1 - + Spectrum 0	- + Sequen	ntial 🔘 Individual	Cancel Select	
7			Fit Cancel		

iii. After all the workspaces added, there are two options for fitting:

- Sequential fit the parameters of a previous fit are used for every new fit.
- Individual fit the parameters of the initial fit are used for every new fit.

SequentialFit											
Par	ame	eter f0.A0			▼ Curv	e Type	Line 👻				
Log Value HB2C:SE:SampleTemp 💌											
Plot against log Pass workspace index to function											
	Cre	eate Output 🗌 Ou	utput Con	nposite Meml	bers 🗌 Cor	nvolve M	lembers				
In	put										
		Workspace/File	Period	Spectrum	WS Index	Range	e Add workspaces				
	1	output_th1		-1	0		Add workspaces				
	2	output_th14		-1	0		Add files				
	3	output_th10		-1	0		Delete				
	4	output_th11		-1	0		Delete				
	5	output_th12		-1	0						
	6	output_th13		-1	0		_				
	7	output_th15		-1	0						
	8	output th16		-1	0						
	Peri	iod 1 -	• +	Spectrum 0	-	+	 Sequential Individual 				
?							Fit Cancel				

iv. After all the adjustments are done, click "Fit".



7) In order to view, go to the workspaces and find the file "**Name_of_your_file_res**". Right click on it and select "**Show data**".

Workspaces	@ × E(Scroll righ	nt to se	e all th	ne data	a 📕				
Load 🔻 Delete	Clear +									
Group Sort 💌	Save 🔻			ou	tput_th1_res	- Mantid			- 0	×
Group Sort +	Save	HB2C:SE:SampleTemp	f0.A0	f0.A0_Err	f0.A1	f0.A1_Err	f1.Mixing	f1.Mixing_Err	f1.Intensity	1
Filter Workspaces		1 26.3	-0.355403	0.0021497	0.00639099	1.96948e-05	0.999759	0.00243315	3.89922	0
· · · · · · · · · · · · · · · · · · ·		2 338.6	-0.157697	0.0129507	0.00518613	0.000117625	0.999996	0.0159312	3.17916	0
Workspaces		3 238.6	-0.157697	0.00886784	0.00518613	8.05476e-05	0.999998	0.0110793	3.17916	0
output_th1_Normalise	dCovarianc	4 263.6	-0.157697	0.0105302	0.00518613	9.56457e-05	0.999999	0.013083	3.17916	0
multiple.interpretation of the second sec		5 288.6	-0.157697	0.011412	0.00518612	0.000103649	0.999999	0.0141233	3.17916	0
		6 313.6	-0.157697	0.0122863	0.00518612	0.000111601	1	0.0151688	3.17916	0
output_th1_res		7 363.6	-0.155523	0.0138426	0.00520729	0.000125711	0.99921	0.0171714	3.14066	0
autout the Morkense	Show Data	8 388.6	-0.152799	0.0151831	0.00523094	0.000137775	0.99996	0.0190298	3.08904	0
Maarithma	Show History	9 413.6	-0.149898	0.0166933	0.00524563	0.000151336	0.999948	0.0211472	3.02919	0
Algorithms		10 463.6	-0.143626	0.0212067	0.00527499	0.000191974	0.999879	0.0274171	2.94043	0
	Rename	11 438.6	-0.143631	0.0187982	0.00527494	0.000170135	0.999948	0.0243159	2.94046	0
Execute LoadWAND	C N.Y	12 38.6	-0.17449	0.00293032	0.00499095	2.66389e-05	0.999497	0.00444202	2.75392	0
A duith muchin	Save NeXus	13 488.6	-0.0433525	0.0243841	0.00435959	0.000220417	0.999988	0.0322581	2.89178	0
 Arithmetic CorrectionFunctions 	Delete	1/ 513 5	-0 0415081	0.0784147	0 00437776	0 000256972	0 99987	0 0373996	7 RAAR7	n

8) To plot it, select a column, right click on it and select an option. The Sample Log values are automatically selected as x-values.

tv f1.Intensit	f1.Intensit	a f1 Mixina Frr f	f1.M	f0.A1_Err	f0.A1	f0.A0_Err	f0.A0	HB2C:SE:SampleTemp	
	Line	t 🕨	0.	1.96948e-05	0.00639099	0.0021497	-0.355403	26.3	1
th Y Errors	Line with	ру	0. 🖸	0.000117625	0.00518613	0.0129507	-0.157697	338.6	2
	Scatter	as X	0.	8.05476e-05	0.00518613	0.00886784	-0.157697	238.6	3
with Y Errors	Scatter v	as Y	0.	9.56457e-05	0.00518613	0.0105302	-0.157697	263.6	4
Symbol	Line + S	error for Y	0.	0.000103649	0.00518612	0.011412	-0.157697	288.6	5
0.0177891	17916	as None	1	0.000111601	0.00518612	0.0122863	-0.157697	313.6	5
0.0199073	4066	tistiss on Columns	0.	0.000125711	0.00520729	0.0138426	-0.155523	363.6	7
0.0217315	8904	tistics on Columns	0.	0.000137775	0.00523094	0.0151831	-0.152799	388.6	8
0.0237191)2919	e Selected	0.	0.000151336	0.00524563	0.0166933	-0.149898	413.6	9
0.0299465	4043	ow All Columns	0.	0.000191974	0.00527499	0.0212067	-0.143626	463.6	10
0.0265678	4046	t Ascending	0.	0.000170135	0.00527494	0.0187982	-0.143631	438.6	11
0.00456012	75392	t Descending	0.	2.66389e-05	0.00499095	0.00293032	-0.17449	38.6	12
0.0347758	.89178	0.0322581 2	0.999	0.000220417	0.00435959	0.0243841	-0.0433525	488.6	13
0.0396144	.84487	0.0373996 2.	0.999	0.000256972	0.00437776	0.0284142	-0.0415081	513.5	14

9) To save the data, go to Algorithms and execute "**SaveASCII**" to save the table in a comma separated file.

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WAND ² Event Filter and Sequen	tial Fit manual	
		Page 13 of 13
Algorithms	Saves a 2D workspace to a ascii file.	
Execute SaveAsc	InputWorkspace output_th1_res Filename	C Browse
Arithmetic SaveAscii SaveAscii CorrectionFunctions	WorkspaceIndexMin WorkspaceIndexMax	
▶- Crystal	SpectrumList	
▶ - DataHandling ▶ - Diagnostics	Precision ScientificFormat	
Idle. Details	✓ WriteSpectrumID CommentIndicator # ? Keep Ope	n Run Close

Type in the "**Name_of_your_file_res**" as the Input Workspace. Then click on Browse, name the file and click on Save.

Name	filtered_data		Save
			C7
		Size	Modified \bullet
			14 Jun
			14 Jun
			15 Jun
			17 Jun
			17

10) If you want to download these files for use with Rietveld refinements on your local PC/laptop, you can either use a server storage service like Google drive or Dropbox, or download using FileZilla or WinSCP (link on the webpage).